Indoline, 1-(2-pyridylmethyl)-20948-77-0 | DTXSID40175125

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 8.00

Global applicability domain: Inside

Local applicability domain index: 9.83e-01

Confidence level: 8.07e-01

Nearest Neighbors from the Training Set

Image not found

2,4,5-Trichlorobiphenyl

Measured: 8.00 Predicted: 8.15

Image not found

2,4',6-Trichlorobiphenyl

Measured: 7.72 Predicted: 7.94

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1,3,5,8-Tetrachloronaphthalene

Measured: 8.28 Predicted: 8.21

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1,3,5,7-Tetrachloronaphthalene

Measured: 7.90 Predicted: 8.21